Engineered Solutions through Simulation Insights

HEN it comes to finding solutions to tough, national security challenges, scientists and engineers cannot always rely on experiments to ferret out the information they need. Many experiments would simply be too large, dangerous, or expensive to be feasible, leaving technical experts to reconcile knowledge gaps by other means.

Simulations have become an increasingly valuable tool, helping researchers better understand experimental results and bolstering confidence in solutions they develop for various problems. (See the box on p. 28.) Computational engineers at Lawrence Livermore focus most of their efforts on issues related to national security. Bob Ferencz, a group leader in Livermore's Engineering Directorate, says, "We use simulation to evaluate high-consequence scenarios that we cannot easily test because of experimental costs or other concerns."

For example, Laboratory engineers are applying the hydrostructural analysis codes ALE3D and ParaDyn to simulate physical events that last only a few microseconds to several hundred milliseconds and involve large material deformations, high strain rates, and strong shocks. ALE3D and ParaDyn can offer insight into the detonation process of high explosives and material collisions at hypervelocities, in which materials travel 2 kilometers or more per second. By continually developing and improving these computational methods, Laboratory scientists and engineers are providing decision makers with reliable data for evaluating national security efforts.

An Unexpected Twist

ALE3D is a multiphysics-based numerical simulation tool for analyzing the fluid and elastic, or plastic, response of materials under extreme conditions. The finite-element code applies arbitrary Lagrangian–Eulerian (ALE) techniques to simulate material response on an unstructured grid. With funding from the Department of Homeland Security's Science and Technology Directorate, a Livermore team led by computational engineer Lee Glascoe used the code to evaluate techniques that limit damage to underwater structures from destructive blasts.

Underwater structures often suffer more severe damage from a blast than those surrounded by air because water has a higher density and is more incompressible than air. As a result of this tamping effect, the energy released during an explosive detonation couples to the structure more efficiently. "When trying to protect a structure from a blast, creating an appropriate standoff distance is normally the most inexpensive solution," says Glascoe. "However, for this particular scenario, space was limited. The question we had to answer was what to do when the standoff distance is so tightly constrained."

Using ALE3D, Glascoe and his team analyzed methods for diffusing explosive energy coupled to a vertical, partially submerged structure in a restricted space. The researchers simulated several possible tactics, specifically, placing an air gap

or a matrix of air-filled media between the explosive source and the structure. In experiments, they used different-sized, water-filled aquariums fitted with aluminum plates to represent the structure and subjected each one to controlled blasts from explosives. When they analyzed the data, the results seemed rather strange. "At first, we thought there might have been an error in the data acquisition," says Glascoe.

With an air gap in front of the plate, the plate unexpectedly became deformed over one area. The researchers hypothesized that a small, previously unaccounted-for water layer between the charge and air gap could be to blame. "We then ran ALE3D simulations to better understand the results and obtained the same focused deformation." Instead of dispersing the energy from the shock wave, the water-tamped explosive projected the intervening water as a jet toward the plate. Conversely, tests with a matrix of air-filled tubes scattered the shock wave and prevented water jets from forming. Glascoe says, "This relatively heterogeneous material creates an impedance mismatch that disrupts and scatters the blast wave, providing protection across a large threat space."

Glascoe is quick to point out the positives of computational power for understanding complex physics problems and evaluating solutions. "Once we understand the problem well enough to focus on a specific response—plate deformation, for example—we can use advanced sampling techniques to stitch together a comprehensive picture of the anticipated result with fewer simulations," says Glascoe. Carefully analyzing the computational results also helps researchers optimize the design of future experiments. "Smart approaches to simulation save us time and money," he says. The team is now integrating strategies developed in this study into plans for better protecting existing civil structures.

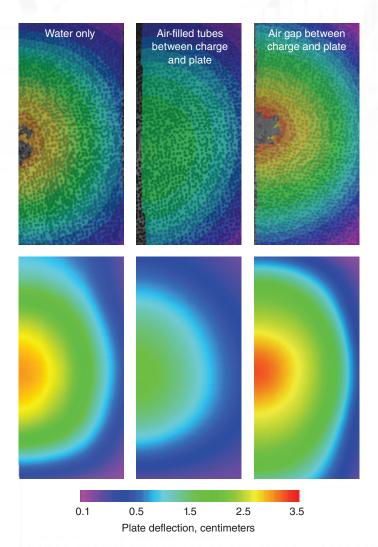
Target Acquired

The Missile Defense Agency (MDA) is responsible for protecting the U.S. and its allies from short- and long-range ballistic missile attacks. Toward this end, MDA's goal is to develop an integrated ballistic missile defense system for neutralizing potential threats. Flight tests of different systems provide valuable data, but they are costly and cannot assess a particular design's effectiveness to all possible threats. MDA is thus working with a team of Livermore engineers to simulate system operations for various threat scenarios. "We bring a comprehensive knowledge of hypervelocity impact physics and of material response in this type of high-rate, high-pressure environment," says Laboratory computational engineer Ed Kokko. "Our physics-based simulation tools coupled with our high-performance computing platforms allow us to provide timely, cost-effective answers to sponsor concerns."

One strategy for neutralizing incoming threats is through a kinetic-kill approach, where an inert projectile, or kill vehicle, engages the incoming threat at a very high speed. MDA system architects are primarily concerned with intercept lethality, that is,

whether the intercept event successfully destroys the threat. The ParaDyn code is well suited for examining such events because it allows engineers to analyze the transient dynamic response of three-dimensional solids and structures. It is especially effective at detailing the interaction between independent bodies, such as the incoming threat and the kill vehicle. "ParaDyn and ALE3D provide us with insight into the time sequence of events during an intercept," says Kokko. "They help us determine the effectiveness of the kill vehicle in neutralizing a threat payload for a range of conditions."

OUA SISKS



Experiments (top row) and hydrodynamics simulations (bottom row) of a structure's response to a water-tamped explosion compare the effects of pure water tamping (left) with mitigation by a matrix of air-filled tubes (middle) or the presence of an air gap (right). Placing the matrix between the blast and an underwater structure improves structural protection over a large threat space.

60 Years of National Service

Accelerating Scientific Discovery

Supercomputing systems continue to grow in size and processing speed. With these more powerful resources, scientists and engineers can examine complex physical processes in greater detail.

Advanced simulation capabilities have been crucial to the National Nuclear Security Administration's Stockpile Stewardship Program, instituted in 1992 to ensure the safety, security, and reliability of the nation's nuclear weapons stockpile without underground testing. Computational codes such as ParaDyn and ALE3D stemmed from the needs of stockpile stewardship, and code enhancements continue to support the missions of the Departments of Energy and Defense and other government agencies.

"Simulations help us better understand the physics of a particular problem so we can develop a more robust set of solutions," says Rob Sharpe, a division leader in Livermore's Engineering Directorate. "Going forward, advances in computational engineering will offer different methods to optimize and assess system design and to provide solutions in a more systematic manner, which ultimately will accelerate scientific discovery." The natural coupling of ParaDyn and ALE3D into an embedded grid is a prime example of how Livermore

computational engineers are using their expertise to further simulation capabilities. "By combining techniques and using more precise variables, we can get closer to seeing the true physics involved in a scenario, which in turn will change the way we design and build systems," says Sharpe.

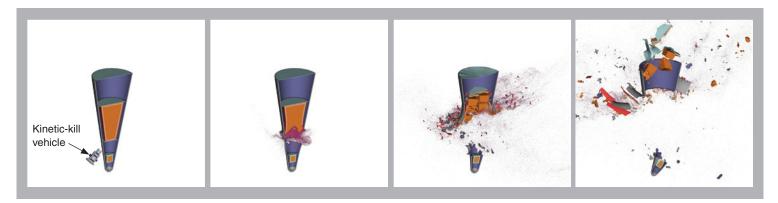
The Laboratory typically invests in creating simulation tools when no thirdparty source will suffice or when the tool is considered essential to fulfilling programmatic requirements. Such efforts have already paid off in the design and assessment of complex mechanical and structural systems as well as in highfidelity modeling of electromagnetic phenomenon. According to Bob Ferencz, an Engineering group leader, development of code capabilities arises from a focus on specific applications but can be extended to meet the needs of sponsors in addressing broader concerns, especially in support of national security.

While simulation cannot exist in the total absence of experimentation, the continued "virtualization" of engineering assessment and design certification is inexorable. Sharpe points out that further enhancements in computational engineering will be extremely valuable for

uncertainty quantification assessments, which focus on measuring how accurately simulations predict the outcomes that are most likely to occur. (See *S&TR*, July/ August 2010, pp. 12–14.) "Improved computing ensures that we're asking the right questions of the simulations to get the right answers," he says. The models support more focused experiments, the results of which then inform the next set of models, providing higher confidence in the overall data.

The expertise developed by the Livermore staff and the continued investment in computing resources position the Laboratory to further enhance its capabilities in computational engineering. "Our accomplishments in engineering simulation also help the Laboratory expand collaborations with the public and private sectors," says Ferencz. "In addition, these techniques and tools could lead to new avenues of research and experimentation." Sharpe adds that the rapid increases in supercomputing power and improved algorithms, combined with high-fidelity data and an expanded knowledge base, are being applied to solve some of the nation's most challenging problems. Sharpe says, "We're bringing science to bear in a practical way."

S&TR September 2012 Computational Engineering



ParaDyn helps engineers analyze the mechanical interaction between independent bodies. In this theoretical missile defense scenario, the code simulated a kinetic-kill vehicle as it impacts a reentry threat at hypervelocity and the resulting breakup.

Engineers are also interested in understanding how the interceptor and threat break into pieces on impact. Livermore code developers have enhanced ParaDyn with advanced material models and improved numerical techniques to more accurately simulate an intercept event. Computational engineers, including Kokko, are working with the revised code to provide detailed information about the debris scene.

Simulation codes such as ParaDyn offer a cost-effective approach for system-level analysis at a time when expensive, full-scale experiments are becoming more difficult to stage. "We have been focused on establishing a basis of confidence in our modeling methodology to verify that simulations compare well with experimental results at the fundamental, component level and for scaled and full-scale systems," says Kokko. Confidence in simulation results is essential to sponsors who rely on the data to make critical decisions, and the widespread adoption of physics-based numerical codes for analyzing such events makes this an ever-more important effort.

Two Codes Team Up

The old adage "two heads are better than one" can apply to computer codes as well. In a project initially funded through the Laboratory Directed Research and Development Program and led by Livermore engineer Mike Puso, new algorithms were developed to combine codes such as ALE3D and ParaDyn into a united capability. "This work focused on creating a fundamental numerical technology that allows multiple codes to attack different parts of the same problem," says Ferencz. "In this way, a broader range of problems can be solved with higher fidelity." The result is an embedded-grid numerical code in which two meshes overlap and are processed together by two distinct simulation codes.

Successful demonstration of the technology led to an exciting partnership between the Laboratory and the Blast Protection for Platforms and Personnel HPC [high-performance computing] Software Applications Institute, sponsored by

the Department of Defense's High Performance Computing Modernization Program and headed by the Army Research Laboratory. The institute has embarked on a six-year program to develop a suite of tools for analyzing high-explosive blasts and mitigating the effects on military vehicle platforms and personnel. Says Ferencz, "Our primary contribution is to provide a simulation capability that enables efficient, accurate analysis of these complex problems."

Building Confidence in Simulated Solutions

The capabilities provided by Livermore's high-performance computers enable computational engineers such as Ferencz, Glascoe, and Kokko to validate codes quickly and efficiently and apply those calculations to many classes of problems. "Our advanced computing resources often exceed industrial capabilities," says Ferencz. "As a result, we can run multiple, detailed simulations simultaneously with much shorter turnaround times."

When researchers can obtain complex results in days instead of weeks, they can also dedicate more time to understanding an input parameter's effect on code sensitivity. "Sensitivity studies are an important part of the analysis process," says Kokko. "Investigating how results vary with assumptions across many scenarios helps us build confidence in our results."

Studies that help validate the performance of computational codes are propelling viable, novel solutions to some of the nation's greatest challenges. Says Kokko, "We have a responsibility to our sponsors to deliver accurate, reliable data so they can confidently make decisions regarding our national security."

—Caryn Meissner

Key Words: ALE3D code, arbitrary Lagrangian–Eulerian (ALE) technique, computational engineering, embedded grid, ParaDyn code.

For further information contact Bob Ferencz (925) 422-0571 (ferencz@llnl.gov).